=> file reg

FILE 'REGISTRY' ENTERED AT 19:15:58 ON 15 NOV 2007

chain nodes:

72 73 74 75 76 77 78 79 80 81

ring nodes:

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23

24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48

 $49\ 50\ 51\ 52\ 53\ 54\ 55\ 56\ 57\ 58\ 59\ 60\ 61\ 62\ 63\ 64\ 65\ 66\ 67\ 68\ 69\ 70\ 71$ chain bonds :

2-7 3-8 4-9 5-10 6-11 37-78 37-79 40-76 40-77 43-74 43-75 46-72 46-73 49-80 49-81

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6 7-12 7-16 8-17 8-21 9-22 9-26 10-27 10-31 11-32

11-36 12-13 13-14 13-49 14-15 14-51 15-16 17-18 18-19 18-46 19-20 19-48 20-21 22-23

23-24 23-43 24-25 24-45 25-26 27-28 28-29 28-40 29-30 29-42 30-31 32-33 33-34 33-37

```
34-35 34-39 35-36 37-38 38-39 38-60 39-63 40-41 41-42 41-56 42-59 43-44 44-
45 44-52
45-55 46-47 47-48 47-68 48-71 49-50 50-51 50-64 51-67 52-53 53-54 54-55 56-
57 57-58
58-59 60-61 61-62 62-63 64-65 65-66 66-67 68-69 69-70 70-71
exact/norm bonds:
13-49 14-51 18-46 19-48 23-43 24-45 28-40 29-42 33-37 34-39 37-38 40-41
43-44 46-47 49-50
exact bonds:
2-7 3-8 4-9 5-10 6-11 37-78 37-79 40-76 40-77 43-74 43-75 46-72 46-73
49-80 49-81
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 7-12 7-16 8-17 8-21 9-22 9-26 10-27 10-31 11-32
11-36 12-13 13-14 14-15 15-16 17-18 18-19 19-20 20-21 22-23 23-24 24-25 25-
28-29 29-30 30-31 32-33 33-34 34-35 35-36 38-39 38-60 39-63 41-42 41-56 42-
59 44-45
44-52 45-55 47-48 47-68 48-71 50-51 50-64 51-67 52-53 53-54 54-55 56-57 57-
58 58-59
60-61 61-62 62-63 64-65 65-66 66-67 68-69 69-70 70-71
```

Match level:

- 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
- 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom
- 19:Atom 20:Atom 21:Atom
- 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom
- 30:Atom 31:Atom 32:Atom
- 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom
- 41:Atom 42:Atom 43:Atom
- 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom
- 52:Atom 53:Atom 54:Atom
- 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom
- 63:Atom 64:Atom 65:Atom
- 66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:CLASS 73:CLASS
- 74:CLASS 75:CLASS 76:CLASS
- 77:CLASS 78:CLASS 79:CLASS 80:CLASS 81:CLASS

L1 STRUCTURE UPLOADED

=> s 11 sss sam

L2 1 SEA SSS SAM L1

=> s 11 sss ful

L3 6 SEA SSS FUL L1

=> file hcaplus uspatfull

FILE 'HCAPLUS' ENTERED AT 19:16:50 ON 15 NOV 2007

FILE 'USPATFULL' ENTERED AT 19:16:50 ON 15 NOV 2007

=> s 13 .

FILE 'HCAPLUS'

L4 7 L3

FILE 'USPATFULL'

L5 4 L3

TOTAL FOR ALL FILES

L6 11 L3